Computational Simulations of Solid Oxide Fuel Cells

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Summary

Scientists and researchers at Sandia National Laboratories and Ford Research Center have developed and tested an advanced parallel computational capability to simulate hydrogen (H_2) and methane (CH_4) solid oxide fuel cells (SOFC). The simulation code is an extended version of the **MPSalsa** transport / reaction code developed partially under DOE MICS funding. This unique research simulation code employs advanced finite element (FE) methods to numerically solve the governing fluid flow equations with associated thermal energy and mass transfer along with non-equilibrium chemical reactions in complex geometries. An additional electric potential equation, along with the appropriate electrochemical interface conditions, is used to model the voltage potential and provide electric current density information. These equations form a strongly-coupled, highly nonlinear system of equations. The FE approximations to these systems can require the solution of millions of equations in millions of unknowns for the fluid velocities, hydrodynamic pressure, temperature, chemical species and the electrical potential. The computational solution of these systems of equations is very difficult and requires advanced numerical mathematics and computational techniques that can take advantage of large-scale parallel supercomputers. To solve these equations the **Aztec** library, which provides advanced parallel iterative solvers and preconditioners is used. This library was also developed concurrently with the MPSalsa code through MICS funding at Sandia National Laboratories. Previous attempts at robustly solving large-scale simulations of these SOFC systems with computational codes based on state-of-the-science (decoupled) solution methods were unsuccessful. The MPSalsa simulation code has been demonstrated to be highly scalable to thousands of processors.

Intuitively, SOFCs are conceptually similar to batteries. However the SOFC is an open system where chemical reactants flow through the cell. The fuel (typically hydrogen, H_2, or methane, CH_4) is oxidized (burned) at the anode with oxygen ions that are conducted across a solid electrolyte. Heat and electrons are given off in the reaction at the anode (negative potential) and are used to provide the electrical power. Reactions at the cathode (positive potential) combine oxygen (from air) and the electrons returning from the external circuit to form the oxygen ions.

Our current studies of H_2 based SOFCs have detailed calculations for chemical/electrical conversion, non-isothermal effects due to species conversion and Joule heating, and a thermal stress analysis. An example of an axi-symmetric simulation for a bench-top experimental H_2 based planar SOFC is presented in Figure 1 (a).

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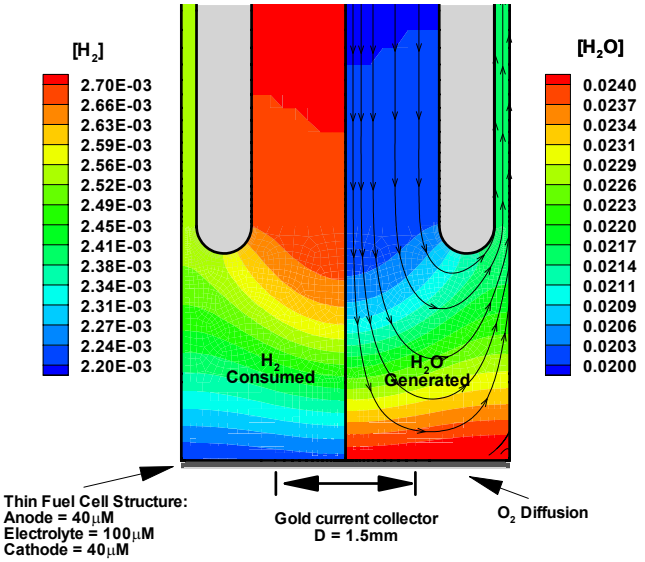

Figure 1(a). Contours of H_2 and H_2O Concentration.

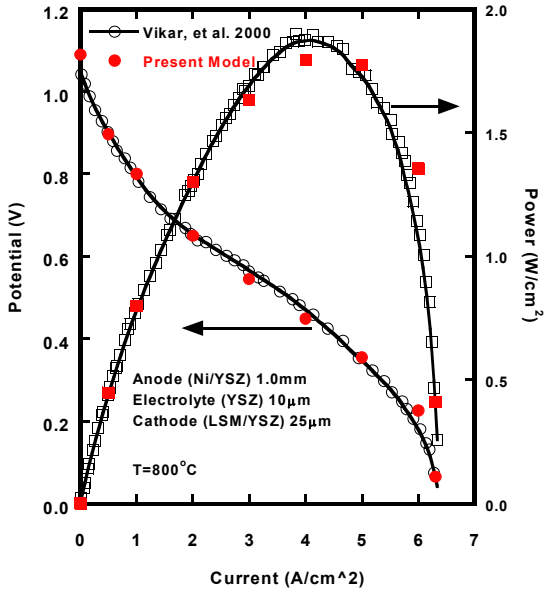

Figure 1(b). A comparison of simulation and existing experimental results for H_2 SOFC.

In Figure 1(b) results are presented for a similar geometry in which the current-voltage curve is compared to experimental measurements available in the literature.

Based on present fuel technologies, it would be desirable to use a hydrocarbon based fuel source in transportation applications. Present 3D simulations are focused on internal reforming of hydrocarbons in SOFCs with initial studies focusing on CH_4 as a model fuel. Using this approach, CH_4 is not burned (oxidized) directly but is, instead, reformed in an endothermic (heat requiring) reaction over a catalytic surface. This reaction produces H_2, and carbon-monoxide (CO). The H_2 and CO are then oxidized in an exothermic (heat producing) reaction in the SOFC to power the electrical system. This partial oxidation of CH_4 and the use of the products of the reforming reactions (H_2 and CO) in the SOFC can be used to more effectively control the thermal energy production of the fuel cell and thermal stress distribution during operation.

Currently this strongly-coupled simulation capability is now being used to explore the highly nonlinear space of solutions in which these systems must operate. In the future similar simulation and solution techniques, used in combination with optimization-based algorithms, can be used to further refine the design of such complex systems.

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